

Process innovation through Integration approaches at multiple scales: a perspective

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Abstract Process innovation can be efficiently enabled by considering it as a holistic procedure, which applies integration—starting from molecules and extending through process tasks, unit operations, plant-wide and finally at enterprise level. It is only through such a comprehensive approach that truly breakthrough process innovations are possible and realisable in a highly competing and enormously complex system environment with multiple counter balancing objectives.

Introduction

The most essential function of process innovation is to unveil, investigate and finally address all inherent complexities within the boundaries of a process system. The endeavour is challenging (Klatt and Marquardt 2009) in the sense that the fundamental chemical and physical transformations at the molecular level should be realised through process tasks within unit operations that are part of a wider super system, which is usually the plant. Nowadays, the interactions among multi-plant entities have attracted significant attention by exploring integration at enterprise level. It is, therefore, the role of integration to

exploit synergies and identify constraints (Klemeš 2013) among the various levels of system abstraction. Various process levels can be distinguished as follows:

- Molecular level
- Process task and unit operation level
- Plant-wide level
- Enterprise level

At the molecular level, computer-aided molecular design (CAMD) has been proved to achieve significant benefits for the entire process (Papadopoulos et al. 2013). CAMD aims to synthesise molecules so that the working streams possess the essential characteristics and properties that would facilitate the intended process tasks. CAMD applications and their integration with a process task level analysis have successfully identified optimum Organic Rankine Cycle single fluids or mixtures (Papadopoulos et al. 2010), CO₂ capture solvents via absorption to name a few.

At the process task and unit operation level, process synthesis has played the most decisive role in the systematic identification of efficient flowsheet configurations. Interactions of molecular level innovation with process tasks level analysis result in novel process systems of enhanced potential. Modelling and model-based optimisation are the main tools for innovative process equipment for intensified phenomena-driven solutions (Kenig 2008). Modelling has enormously accelerated the design procedure by eliminating the need of multiple costly and time-consuming experiments. Eventually, a limited number of targeted experiments are now required for proving complex concepts combining transport phenomena, reaction kinetics and thermodynamics.

At the plant-wide level energy and resources (e.g., water and raw materials) integration, (Varbanov and Klemeš

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2011) highlights the contribution with the highest impact in modern process industry. However, the links connecting decisions at the molecular level through the process tasks and unit operations levels may have a dramatic effect on the performance at the plant-wide integration level. Therefore, it is only through an approach, which incorporates integration at multiple levels that such a benefit can be directly realised in innovative process designs.

The enterprise level includes the supply chain of products and raw materials as well as financial considerations (Láinez et al. 2009) in addition to the production activities. Considering the need for greater competitiveness and true sustainability, companies are seeking synergies among themselves for shared infrastructure and more efficient resource utilisation through complementarity of needs (the waste from one player can become a useful component for another player).

A good example of simultaneous consideration of all these process levels is the CAPSOL project (2012). Its consortium has implemented a levelwise integration approach for the development of solvent-based post-combustion CO₂ capture processes. A small set of potentially efficient solvents in the CO₂ capture process has been identified using CAMD techniques that were subsequently used in the design optimisation of a complete process flowsheet. Furthermore, innovative process equipment can be manufactured, tailored to the nature of the selected solvents. The overall performance is finalised through a series of heat integration studies for reference power plants. In a recent work, Papadopoulos and Seferlis (2009) incorporated extractive solvent selection with process design optimisation with the explicit consideration of controllability properties of the overall system.

This article reviews a collection of new developments put into the context of other recent works in the key fields of Process Integration Tools for Sustainable Production, Process Development for Intensified Production, Waste Management and Emissions Control, and Biorefinery and Biomass Utilisation Technologies.

Process integration tools for sustainable production

The success of Process Innovation through Process Integration relies heavily on the development of efficient and reliable tools (Klemeš et al. 2013). Such tools utilise first principles-based mathematical or data-driven models along with methods such as process synthesis and design, real-time optimisation, automatic control, heat integration (Klemeš and Kravanja 2013) and so forth. The designer can subsequently exploit the process integration tools to reach the appropriate process solution within the predefined set of performance criteria. The variety of available tools and

their potential implementation in process systems enable the quick development of new processes and the retrofitting of existing ones. Energy and power generation targeting, energy indicators monitoring through data-driven approaches, computational fluid dynamics and simulation approaches as well as decision-making tools using a logistic optimisation provide excellent examples of recent developments (Kravanja 2012) on process integration tools.

Sun et al. (2014) have extended Total Site Pinch Analysis with revisiting the Site Utility Grand Composite Curve (SUGCC) (Klemeš et al. 1997) that enables the targeting of heating and cooling as well as potential shaft power generation through steam expansion. The SUGCC is more appropriate for understanding the interactions between process and utility systems as it explicitly addresses both energy and power targets along with steam cascades. SUGCC offers an efficient visualisation tool for the conceptual design and optimisation of the utility system. It allows the identification of cogeneration potential and the detection of improvements in the overall energy requirements by suitable process modifications considering their direct impact on the utility system.

Abonyi et al. (2014) employ a goal-oriented time-series segmentation technique that automatically selects plant data for energy use at various operating conditions in order to build efficient data-driven targeting models for energy demand estimation. The analysis of key energy indicators allows the evaluation of process efficiency at different operating regimes. Based on reliability of the extracted knowledge, realistic targets for such energy indicators can be determined. The collection of historical data over different operating regimes is accompanied with the development of regressed prediction models. Partial least squares technique has been used in the detection of the different operating regimes from which the data were gathered. The technique has been successfully applied to a heavy naphtha hydrotreater and a catalytic reforming process.

Egedy et al. (2014) investigated the implementation of computational fluid dynamics (CFD) tools for the efficient modelling of a chemical reactor for the dissolution of electrical waste such as computer memory and motherboards and the recovering of precious metals. A hybrid CFD compartmental approach was developed to describe the dissolution process in the leaching reactor that consisted of a rotating perforated drum. Navier–Stokes equations were used to model the momentum balance in the reactor along with rotating wall boundary specifications. CFD modelling allowed the calculation of the hydrodynamic behaviour within the reactor under various rotating speeds and the dissolution of the precious metals. The validated model has been used for the optimisation of the

operating conditions such as the rotating speed and the initial reagent concentration.

Chettouh et al. (2014) employed simulation models in order to accurately predict phenomena in industrial fires. The main characteristic of such models is the large amount of uncertainty that is involved arising from lack of knowledge about the prevailing meteorological inputs, the use of difficult to verify assumptions about the diffusion of emission, stochastic nature of plume dynamics and the lack of understanding the emission generation mechanism. A Monte Carlo simulation approach has been used that enabled the calculation of sensitivity factors on the NO₂ dispersion. The obtained simulation results showed that the viscosity coefficient and the wind speed are the parameters with the greatest impact on NO₂ concentration near the source of the fire. The sensitivity pattern changes at areas further away from the source of fire with the wind speed and the initial concentration becoming the most important parameters.

Šomplák et al. (2014) developed a novel tool for logistic optimisation and capacity sizing for municipal waste management. Basically, the producer of waste makes a decision about its future municipal waste treatment strategy considering the cost of transportation waste to the waste-to-energy facilities as well as any other environmental taxation that is included and reflected in the gate fee. Even though the concept is simple, the tools take into consideration in full scale the availability of transportation routes through a properly selected incidence matrix along with the associated costs and capacity limits. In addition, the developed tool incorporated the uncertainty emerging from the variation of the gate fee at individual facilities. A stochastic programming approach allowed for the statistical analysis of the results. The tool has been successfully used for the planning and spatial allocation of new waste-to-energy facilities in a region of the Czech Republic.

Data reconciliation plays a key role in the monitoring of industrial plants. It is used for early detection of critical events and eventual process failures and as such is an essential component of clean technology processes. Vociante et al. (2014) propose a statistical data reconciliation procedure using information about the structure of the random errors of the measured flow rates. The proposed method is illustrated with a numerical example able to reduce the measured value discrepancies down to 5–10 % for the most variables and to identify gross errors in the system.

Process development for intensified production

Process Development for Intensified Production is certainly a key to the development of economical and sustainable

solutions (Klemeš and Varbanov 2013). Intensification aims at combining the beneficial interactions of multiple process tasks and transformations within a unified envelope. Characteristic examples are membrane reactors where thermodynamic limitations are circumvented due to the preferential separation or the distributed feeding of products and reactants. Similarly, the acceptance of new process technology encompassing intensified production schemes by industry requires the execution of experimental studies under conditions prevailing at the industrial site for which the technology is intended. The development of mini-plants suitable to accommodate industrial process streams accelerates the validation of the theoretical tools and the fine-tuning of the proposed technology facilitating the industry acceptance procedure.

Patcharavorachot et al. (2014) applied a membrane reactor to the oxidative coupling of methane process in order to prevent deep oxidation of a desirable ethylene product. The membrane reactor enables distributed feeding of the oxygen along the reactor length resulting in improved selectivity. The operation optimisation of the membrane reactor is achieved with the use of a mathematical model of reactor that incorporates the complete mass and energy balances coupled with a detailed kinetic reaction mechanism. The membrane reactor performance is assessed based on the achieved methane conversion, C₂ selectivity and C₂ yield. The simulation results indicated that C₂ production is enhanced at high temperature and low methane to oxygen feed ratio. The optimum operating conditions have been calculated using a response surface methodology.

Günther et al. (2014) proposed a procedure for the adaptation of new technology through testing under conditions encountered in industrial sites. Impurity-free experimental laboratory work has been upgraded to mini-plant scale experiments using a bypass of the actual industrial process streams. The mini-plant experiments along with theoretical studies based on simulation models make possible the development of new process technologies without serious acceptance issues by industry. More specifically, a new reactor technology for the hydrogenation of SO₂ is investigated through the development of an experimental setup installed at the industrial target plant. The experiments verified the selectivity of the catalyst, the stability of the catalyst, the oxygen tolerance of the catalyst and investigated the optimal operating policy. A validated reactor model assisted in the calculation of optimal reactor parameters.

Waste management and emissions control

Sustainability cannot be properly addressed without an efficient waste management strategy. It is widely accepted

that the cost for sustainable operation has multiple return benefits for process industry. The main goal of process systems engineering was not only to offer solutions to the treatment and the disposal of safer waste streams but also to create opportunities for the replacement of raw materials by appropriately treated waste (Fodor and Klemeš 2012). Along these guidelines, life cycle assessment, performance evaluation and optimisation of alternative waste utilisation procedures are essential elements for sustainable production. Furthermore, development in the systematic generation of highly performing flowsheets and the calculation of the specifics in the unit operations performance clearly indicate an advancement in existing technologies.

Margallo et al. (2014) used the life cycle assessment approach to evaluate and compare ash solidification with ash recycling in Portland cement production as a clinker and gypsum substitute. The study showed that the substitution of ash for clinker resulted in the lowest natural resources (NR) consumption and the lowest environmental burdens (EB). The decrease in the clinker substitution percentage generated a higher NR consumption and an increased EB. In ash recycling, the distance between the incinerator and the cement facility is a key parameter in the decision making.

Jecha et al. (2014) investigated the suitability of a catalytic oxidation unit with the use of a Pt–Pd/Al₂O₃ catalyst for volatile organic components (VOC) abatement compared to an existing incinerator. A pilot plant was designed in order to investigate the potential deactivation of the catalyst by solid impurities and to confirm the achieved conversion of VOC and CO. The reactor has been divided into two parts with intermediate cooling by pressurised air to prevent extreme temperature rise that would eventually cause an irreversible damage to the catalyst. The operation of the pilot plant proved the long-term reliability and efficiency of the catalytic reactor as only minor deactivation of the catalyst was observed and the effluent gases met all local emission limits.

Houshfar et al. (2014) studied the emissions formation and release of main ash-forming elements during thermal conversion of biomass fuels at different conditions. The experiments were conducted in a quartz glass reactor under both oxidation and pyrolysis conditions at controlled temperature levels, atmosphere conditions and residence time. A wide variety of biomass compositions have been tested such as torrefied softwood, spruce bark, waste wood, miscanthus and wheat straw. The results indicate the main trends in the ash formation and the emissions as a function of the prevailing conditions and the temperature levels.

Rashidi et al. (2014) aimed at the manufacture of low-cost activated carbon from coconut waste. The activated carbon was then tested for its efficiency in post-combustion CO₂ capture via adsorption. CO₂ adsorption by carbonaceous

materials is attractive due to the low energy requirements, the large availability of the material, the high thermal stability, the low cost and the ease of preparation. A series of activated carbon were prepared and characterised based on their moisture content and surface morphology. A set of adsorption experiments investigated the performance of the coconut activated carbon under variable flue gas stream content and temperature. The coconut-based activated carbon showed quite similar performance to that of commercially available activated carbon materials.

Damartzis et al. (2014) proposed a generalised framework for the optimal design of post-combustion amine-based CO₂ capture processes based on a systemic and flexible equilibrium separation model. Within this context, a column section of adaptive separation capability and functionality serves as the fundamental structural block for the identification of efficient flowsheets. The performance of the separation schemes has been evaluated within a nonlinear optimisation programme. A number of novel flowsheet configurations showed improved performance over the conventional flowsheet for a 30 % wt monoethanolamine aqueous solution. The obtained solutions explored an optimal distribution of process-driving forces through which the overall efficiency of the process can be drastically enhanced.

Petrova et al. (2014) investigated the effects of gas flow maldistribution in different types of gas distribution devices and packings on the velocity profiles in absorption columns. The main indicators used for the assessment of the flow distribution are the dynamic pressure, the maldistribution index (MI) and the coefficient of distribution (CoD). Experiments were performed in a pilot plant. The factors influencing the considered indices are the types of GDD and packings used in installations, the number and dimension of measuring cells, as well as the gas initial velocity and measurement error.

Biorefinery and biomass utilisation technologies

Biomass utilisation is rapidly growing through the development of new concepts (Lam et al. 2011) and process technologies (Rahuet et al. 2013). However, due to the wide range of properties in the various forms of biomass, the processes have to be adapted to the specific cases. It is, therefore, imperative to introduce tailored process system techniques in order to accomplish a systematic design procedure in biomass treatment. The task becomes even more challenging as the biomass transformation mechanisms are sometimes quite uncertain adding to the high-quality variability of the initial feedstock. In addition, multiproduct biorefineries add another dimension to the inherent complexity of biomass utilisation, as several production lines need to be handled simultaneously.

Isaksson et al. (2014) evaluated the influence of varying the biomass pretreatment methods before gasification and Fischer–Tropsch (FT) synthesis—studied widely elsewhere e.g. (Pirola et al. 2014)—crude production on the system performance and greenhouse gas (GHG) emissions. The evaluated system has been proposed as an extension of a pulp and paper mill for utilising its waste streams. The evaluated pretreatment methods include milling, torrefaction and pyrolysis. Their results indicate that it is possible using the excess heat from a FT process with 300 MW_{HHV} biomass input, to replace the bark boiler of a large pulp and paper mill for producing 350,000 t/y bleached paperboard.

García et al. (2014) investigated the application of ultrasound technology to process intensification for the case of dissolution of lignin and hemicelluloses contained in lignocellulosic biomass materials. The dissolution yield was evaluated as a function of the applied ultrasound intensity (power) and duration. The authors have reported optimum lignocellulose dissolution yield maximising the conversion rates, for ultrasound duration of 60 min at 5,000 W.

The concepts for converting a Kraft paper mill into a multiproduct biorefinery have been investigated in (Lundberg et al. 2014) by performing a techno-economic analysis of an example mill. The considered additional products include dissolved pulp (for fibre production), lignin, hemicellulose and electricity for grid export. They have applied Heat Integration and additional process modifications. The authors conclude that the profitability of the explored conversion is very sensitive to the specific capabilities of the mills considered. For the specific mill presented, the authors report annual earnings of the order of 4–8 M€ as a result of the proposed multiproduct conversion.

Another interesting study on the utilisation of biomass waste is presented by Caetano et al. (2014). The authors evaluate the possibility of utilising spent coffee grounds for biodiesel production and potentially for other applications. The investigation has been conducted by means of an experiment using various solvents for extracting lipids from the biowaste. They report that up to 6 wt% can be obtained. Other uses such as fertiliser and as solid fuel have also been studied. A two-step, acid-catalysed, biodiesel production process has been recommended as optimal by the authors.

The sustainability of biodiesel production has been the focus of the work by Liew et al. (2014). The authors emphasise that alongside the technical and energy-yield considerations, additional criteria are important in evaluating the biodiesel production sustainability. They have considered health and safety issues and environmental performance. A systematic framework for assessing alternative biodiesel production pathways during the R&D

stage is presented, employing fuzzy optimisation. The authors report that the most sustainable approaches are production pathways using enzymatic conversion of waste vegetable oil, compared to pathways employing more chemicals or extreme operating conditions.

Hancsók et al. (2014) propose a method for producing bioparaffins in a crude oil refinery. Bioparaffins are suggested as a partial or potentially complete replacement for the fatty acid-methyl-esters contained in the biodiesel. They can be produced using various biowaste raw materials—nonfood vegetable oils, algae oils, etc. This work presents an investigation of advanced Ni-, Mo- and Pt-based catalysts carried out for the production of bioparaffins from different natural triglycerides (oils and fats) and high molecular weight Fischer–Tropsch hydrocarbons. The authors report that reaction yields up to 99 % of the theoretical values, producing oils with bioparaffin content up to 70 % and with very favourable fuel properties.

Finding additional product and revenue streams for sugarcane processing plants and biorefineries is a suitable way for improving their economic performance. Such additional products can be bioactive compounds, which has been researched by Santos et al. (2014). Brazilian ginseng roots were used as model bioactive compounds source. The authors investigated the application of supercritical fluid extraction for obtaining active compounds, also performing thermal integration of the plant. The proposed process is reported by the authors to exhibit higher selective extraction for b-ecdysone from Brazilian ginseng roots, providing an extract with up to a factor of 2 higher than the results obtained in previous studies.

Conclusions

Seeking Process Innovation requires the mobilisation of Process Integration methods and tools at various levels of abstraction initiating from the molecular and moving towards the enterprise level and potentially to multiple enterprises. Specific topics addressed are Process Integration Tools, Process Intensification, Waste Management and Emissions Control and Biomass Utilisation Technologies. They exhibit a strong link along the various levels where decisions need to be made. Important trends can be noticed—especially that Process Integration has developed beyond heat or power integration, into a tool for combined process improvement, in synergy with Process Intensification. New dimensions of sustainability in industry have been also added such as waste management and emissions reduction in utilising renewable and waste materials for production of energy and goods as well as in the cleaner utilisation of fossil sources.

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